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**by Müge Fermen-Coker, Linhbao Tran, and John K. Brennan**

**ARL-RP-0447**

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*A reprint from International Detonation Symposium, 11 April 2010*

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# A Multi-Scale Modeling Framework for Shear Initiated Reactions in Energetic Materials

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**Abstract.** A multi-scale approach for simulating shear initiated reactions in energetic materials is developed. The model utilizes a continuum level shear localization tracking algorithm, a mesoscale modeling approach to obtain a refined thermodynamic state in localized regions, and a sub-grid model to bring the mesoscale level information into the continuum mechanics code in a thermodynamically consistent manner. A particle-based mesoscale method that is capable of exchanging both heat and kinetic energy between particles is employed. The extent of reaction is calculated at the sub-grid level using an Arrhenius reaction rate expression with a dependency on temperature, pressure, and material properties. The sub-grid model also accounts for an energy dissipation process through heat conduction, which is expected for delayed initiation-type problems. The newly developed framework is implemented into an Eulerian wave propagation code. A sample problem is presented as a verification exercise.

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## Introduction

A critical Army mission is to improve predictive technologies for the development of future weapons systems. Requirements of energetic materials for future weapons have become increasingly stringent. It is desired to have high energy density output while simultaneously satisfying Insensitive Munitions (IM) compliance requirements. Shear initiated reactions are an important aspect of lethality, survivability, and vulnerability considerations. The present paper introduces a numerical

framework for simulating reactions in energetic materials due to shear in ballistic applications using a multi-scale approach.

As summarized by Chou et. al [1], mechanical stimulus such as shockwave growth towards self-sustaining reaction depends on the formation of local regions of elevated thermal energy; also referred to as hot spots. For high explosives (HE), one well known mechanism that gives rise to localized hot spots is the formation of shear localizations. Unfortunately, the predictive capability available for modeling such phenomenon in widely used hydrocodes is not sufficiently developed. Therefore, any configuration where there is a reaction due to shear localizations cannot be satisfactorily modeled using these codes. The ability to predict such complex behavior requires an initiation model that

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accounts for sub-grid phenomenon, *i.e.*, a physics-based model, spanning from the molecular scale to the mesoscale to the continuum, such as the approach proposed here. A molecular-mesoscale-continuum approach is necessary to reduce the errors due to assumptions made in the continuum model in estimating the thermodynamic state in each cell.

Under relatively strong shock conditions, sufficient thermal energy is generated locally, ignition occurs, and subsequent chemical energy release results in progressive shock strengthening until detonation conditions are achieved [2]. This shock-to-detonation transition (SDT) process is fairly well understood at a phenomenological level and is based on the theory of hot spot formation such as void collapse, visco-plastic heating, shear banding, frictional heating, etc. A wide variety of approaches have already been published in modeling shock initiation of explosives. Massoni et al published a model for the ignition and growth of a detonation in pressed solid explosives [3]. They described the various phenomena during visco-plastic pore collapse at the microscopic level. They then incorporated the microscopic models into a macroscopic model that reproduces wave propagation and takes into account the various couplings between the microscopic and macroscopic scales. The governing equations were solved using a shock tracking high resolution scheme, in order to avoid numerical smearing of the shock front.

For conditions where a SDT process does not occur, some other form of initiation of an HE leading to an explosion can take place if the material is sufficiently confined. Such analysis was shown by Frey [4], whose study of shear band initiation indicated that both pressure and shear rate were important parameters in controlling runaway explosion. As discussed in another study, the shear localization mechanism could generate a large ignited surface area that may be one of the necessary conditions for shock initiation [5].

Deformation due to shock or impact is a much different process than deformation due to shear induced plastic flow. Compression by shock or impact implies that the atoms or molecules of the

sample are brought into close contact with each other as they get stimulated by the shock wave. Shear induced plastic flow describes a process where dislocations are created and move due to the applied loads. The current paper deals with the initiation of energetic materials specifically due to the latter type of deformation. Therefore, it is necessary to bring the thermodynamic information from the length scale of the material heterogeneities (mesoscale) to the continuum level (length scale of the weapon system). However, it is necessary to do this in a thermodynamically consistent manner and through a robust and practical computational approach.

We introduce a multi-scale approach for simulating shear initiated reactions that span from the mesoscale to the continuum scale. The approach is presented as a preliminary framework. The model is implemented into the CTH hydrocode developed by Sandia National Laboratories, and the results of a verification exercise are presented.

## Multi-Scale Modeling Approach

Unintended ignition of energetic materials due to impact events is likely to occur in localized shear zones, at sliding interfaces, or at the surfaces of collapsing cavities. Predicting the temperature that results from a balance between plastic work, melting, and heat conduction is critical in predicting the time to reaction as well as the type of reaction. Since the information that causes localized hot spots is simply not available at the continuum level, one can either assume a statistical distribution of hot spots, or bring in a refined scale calculation to the continuum level. The current effort attempts to do the latter, using a unique approach that first focuses on the prediction of potential localization zones at the continuum level. The mesoscale data is then introduced through the use of a sub-grid model only for these predicted zones in order to keep the computational cost manageable. A schematic of the overall approach is shown in Figure 1. There are four major steps as follows: (a) generating data using appropriate mesoscale models, (b) converting mesoscale output to continuum input using a sub-grid model, (c) implementing a modified reactive burn model

at the continuum level that uses refined scale temperatures to calculate the extent of reaction, and (d) continuum level simulations.

## Continuum Model

The continuum code used for this study is CTH; an Eulerian wave propagation code under continuing development by Sandia National Laboratories [6]. It can be used to model multidimensional, multi-material, large deformation shockwave physics. A three-step solution scheme is used where the first step is a Lagrangian step in which the cells distort to follow the material motion. The distorted cells are mapped back to the Eulerian mesh during the second step. The third step modifies the database per user input [7]. Finite volume approximations to the conservation of mass, momentum and energy equations are solved in the Lagrangian step.

A numerical framework for nucleating and propagating shear localizations was developed and implemented into CTH by Stewart Silling, first as a two-dimensional ad-hoc model [8], and later as a generalized localization model in three dimensional space (3D), as discussed in [9,10]. When a set of nucleation criteria is satisfied, a shear localization is formed by introducing a Lagrangian tracer particle. As the shear localizations grow and propagate, more tracer particles are introduced provided that the growth conditions are satisfied along the boundary of the localized region in 3D. The localization conforms to local planes of maximum shear as the dynamic event continues, until the growth criteria are no longer satisfied along the points defining its boundary. For the current study, this existing framework is used to track shear localizations at the continuum level. For an energetic material, the consequence of having shear localizations can be ignition, and not limited to simply loss of strength as in metals. Therefore, some additions to the existing framework were required. A new logic is incorporated to calculate the extent of reaction within the localized regions. The reactive burn model can be activated based on the severity of the temperatures achieved as a function of shear rate as well as the heat dissipation from the localized

region. Refined estimates for temperatures are obtained as input from the mesoscale model along the cells that contain shear localizations. Due to lack of proper constitutive models for energetic materials, the initiation criterion for shear localizations is arbitrarily chosen at present to merely test the framework. As energetic materials characterization evolves or as improved mesoscale models become available in the future, the current framework can be updated to incorporate more theoretical and/or empirical work into the decision making process for initiation.

The thermodynamic state of each material in a cell is determined by its own equation of state. The pressure and energy within a cell are then obtained through a mixture rule as follows:

$$\begin{aligned} P(\rho, T, \lambda) &= (1 - \lambda)P_{UR}(\rho, T) + \lambda P_{RP}(\rho, T) \\ E(\rho, T, \lambda) &= (1 - \lambda)E_{UR}(\rho, T) + \lambda E_{RP}(\rho, T) \end{aligned} \quad (1)$$

where,  $\lambda$  is the extent of reaction, UR implies unreacted explosive, and RP implies reaction products. The rate equation for advancing  $\lambda$  in time is modeled as a reactive burn and typically is a function of density, temperature, pressure and the extent of reaction itself:

$$\dot{\lambda} = \frac{d\lambda}{dt} = f(\rho, T, P, \lambda, \dots) \quad (2)$$

## Sub-grid Model & Bridging Scales

Initiation and evolution of chemical reactions within CTH are based on reactive burn models such as Forest Fire (FF), Arrhenius burn (ARB), ignition and growth (IG), and history variable reactive burn (HVRB). For high explosives under shock loading, these reactive burn models are calibrated based on wedge experiments in which the time history or the trajectory of the reactive planar shock is measured as it evolves into a detonation wave. A disadvantage of this approach is that the resulting burn models are only valid for a simple planar shock profile. They would not be able to handle a typical impact scenario where shear localizations dominate.

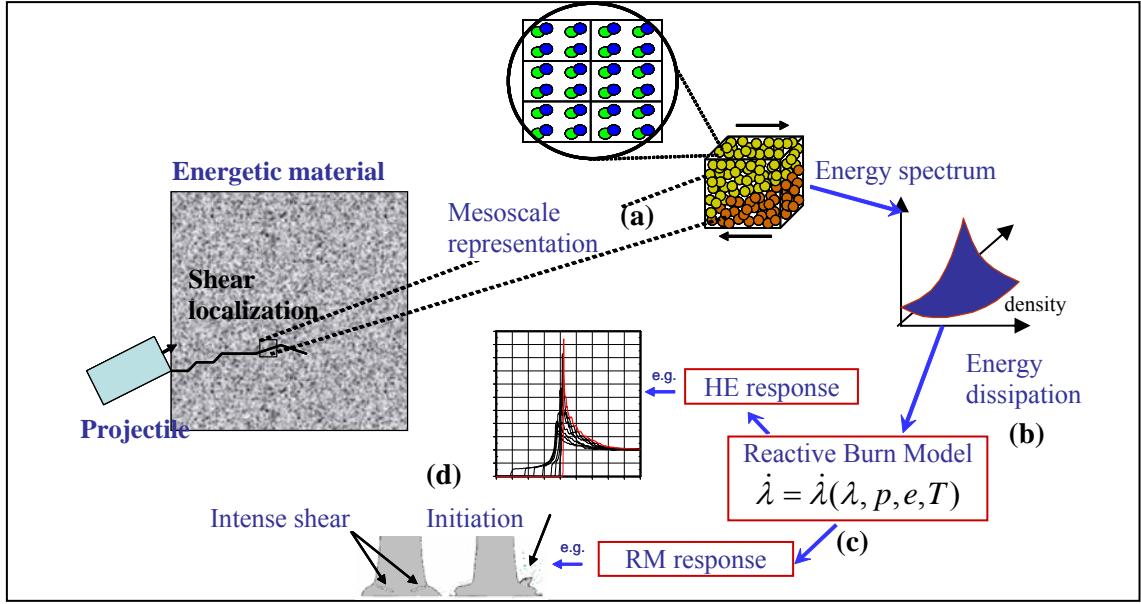


Fig. 1 Schematic of multi-scale shear initiation model.

To bridge the mesoscopic length scale to the continuum length scale, energy and species equations are solved at the sub-grid level within the sheared continuum cells. The initial conditions are provided by mesoscale calculations and the boundary conditions are based on the current thermodynamic state of the continuum cell that contains a shear localization. We employ implicit discretization of the governing equation and attempt to maintain thermodynamic consistency by allowing the calculation of thermodynamic properties only at the continuum level. A general Arrhenius reaction rate expression with dependency on temperature, pressure, and material properties is used.

An important feature of the shear initiation process is the long delay between the time at impact and bulk explosion, which typically can be hundreds of milliseconds. SDT process on the other hand are usually on the order of microseconds. The long delay in reactions can be due to energy competing processes at the microscale. At hot spot locations, e.g. shear surfaces, the possibility of initiation hinges on a balance (or lack thereof) between energy producing mechanisms (visco-plastic work, shear localization, chemical reaction, etc.) and the rate at

which the energy is transported away.

Within each sheared continuum cell, we assume the temperature profile shown in Figure 2. Time dependent equations of temperature and species are described as follows:

$$\rho C \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2} + \Delta H \dot{m}'' \quad (3)$$

$$\rho \frac{\partial \lambda_{sg}}{\partial t} = \rho D \frac{\partial^2 \lambda_{sg}}{\partial x^2} - \dot{m}'' \quad (4)$$

where  $\lambda_{sg}$  is the extent of reaction at sub-grid level, heat of reaction is  $\Delta H$ , diffusion coefficient is  $D$ , and bulk thermal conductivity is  $k$ . The volumetric mass production rate  $\dot{m}''$  is governed by the following Arrhenius type reaction:

$$\dot{m}'' = A \rho (1 - \lambda_{sg}) \exp\left(-\frac{T_a}{T}\right) \quad (5)$$

where  $A$  is the frequency factor and  $T_a$  is the activation temperature. The species diffusion term is assumed to be negligible. The initial conditions are obtained from the continuum and the mesoscale calculations for temperature as follows:



$$\begin{aligned}
T(x,0) &= T_{meso}, & 0 \leq x \leq w_{sb} \\
T(x,0) &= T_{cell}, & w_{sb} < x \leq \Delta L/2 \\
\lambda(x,0) &= 0, & 0 \leq x \leq \Delta L/2
\end{aligned} \tag{6}$$

where  $T_{meso}$  is obtained from mesoscale simulation of a shear process discussed in the following section.  $T_{meso}$  is assumed to be the shear localization temperature.  $T_{cell}$  is the cell temperature calculated by CTH at the continuum level, and  $w_{sb}$  is the assumed width of the shear localization.

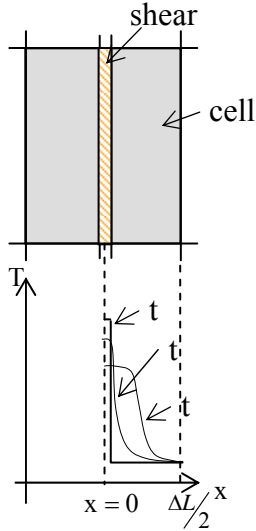


Fig. 2. Illustration of sheared cell and its temperature profiles

The following boundary conditions are used:

$$\begin{aligned}
\frac{\partial T}{\partial x} \Big|_{x=0} &= 0 \\
T(x = \Delta L/2) &= T_{cell}
\end{aligned} \tag{7}$$

Each sheared continuum cell is discretized into sub-domains with five uniform sub-cells within the shear band width, and from there extending out with a given grid expansion ratio. The above governing equations are solved using implicit Euler time integration to ensure stability. The time integration limit at the sub-grid level is

based on the time step from the continuum level.

The resulting extent of reaction profile within each sheared cell is then volume averaged and transferred to the continuum level as a single value extent of reaction for that cell. This extent of reaction is fed back into the continuum level reactive burn model (Eqn. 2) and is used in the equation of state to determine the amount of energy release. This approach ensures consistency in our internal energy calculation.

## Mesoscale Method

The energy conserving version of the dissipative particle dynamics method (DPD-E) is used for the mesoscale modeling portion of this study. DPD-E is a particle-based mesoscale method that conserves both momentum and energy, while allowing the mesoparticles to exchange both viscous and thermal energy [11,12]. In the DPD-E method, the changes with respect to time  $t$  in position  $\{\mathbf{r}_i\}$ , momentum  $\{\mathbf{p}_i\}$ , and internal energy  $\{u_i\}$  of the  $i$ th particle with mass  $m_i$  due to the interaction with the  $j$ th particle can be expressed as

$$\dot{\mathbf{r}}_i = \frac{\mathbf{p}_i}{m_i} \tag{8}$$

$$\dot{\mathbf{p}}_i = \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R \tag{9}$$

$$\dot{u}_i = -\frac{1}{2m_i} (\mathbf{p}_i - \mathbf{p}_j) \cdot (\mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R) + \dot{q}_{ij}^D + \dot{q}_{ij}^R \tag{10}$$

with the requirement that  $\dot{q}_{ij}^D = -\dot{q}_{ji}^D$  and  $\dot{q}_{ij}^R = -\dot{q}_{ji}^R$ ,

where  $\dot{q}_{ij}^D$  and  $\dot{q}_{ij}^R$  are the dissipative and random mesoscopic heat flows, respectively.  $\mathbf{F}_{ij}^C$  is the force due to the conservative interactions, while  $\mathbf{F}_{ij}^D$  and  $\mathbf{F}_{ij}^R$  are the dissipative and random forces, respectively. A particle temperature,  $\theta_i$ , is defined as  $\theta_i \equiv \partial u_i / \partial s_i$ , where  $s_i$  is defined as a mesoscopic entropy. In general, this microscopic state law or *mesoparticle equation of state*,  $\theta = \theta(u)$ , can be determined from atomistic simulations, first-principle calculations, or available experimental data.

Steady planar shear flow was induced by means of the Lees-Edwards boundary conditions [13], in which the simulation box and its images centered at  $(x, y) = (\pm L, 0), (\pm 2L, 0), \dots$ , are taken to be stationary, while boxes in the layer above,  $(x, y) = (0, L), (\pm L, L), (\pm 2L, L), \dots$ , are moving at a speed  $\dot{\gamma}L$  in the positive  $x$  direction, where  $\dot{\gamma}$  is the shear rate. Boxes in the layer below,  $(x, y) = (0, -L), (\pm L, -L), (\pm 2L, -L), \dots$ , move at a speed  $\dot{\gamma}L$  in the negative  $x$  direction. A system under such conditions is subjected to a uniform steady shear in the  $x$ - $y$  plane. Mesoscale look-up tables were generated for a range of densities (1.88-1.90 g/cm<sup>3</sup>) and shear rates ( $10^7$ - $10^9$  s<sup>-1</sup>), where the pressure and the temperature are calculated.

### Coarse-Grained Mesoscale Models

Coarse-graining allows us to simulate phenomena that cannot be simulated using fully-atomistic approaches. The overall strategy is to reduce the number of degrees-of-freedom through simplification of the models used, keeping only those degrees-of-freedom that are relevant to the particular phenomena of interest. Coarse-graining strategies can be categorized as either *bottom-up* or *top-down* approaches. Bottom-up coarse-grain models are built directly from *ab initio* or atomistic simulations, where the atomistic representation is mapped onto the coarse-grain particle. Coarse-grain particle interaction potentials are then derived by applying least-squares approximations to match either the structures or forces of the atomistic and coarse-grain systems. Conversely, top-down coarse-grain models are built by first choosing an analytical potential for the coarse-grain particle interactions, followed by fitting of the potential parameters to either experimental or atomistic simulation observables.

In this work we implement a top-down approach, where the particular form of the potential function is the standard pairwise Morse potential given as:

$$\psi_M(r_{ij}) = \begin{cases} \varepsilon(e^{-2\alpha d} - 2e^{-\alpha d}) & \text{for } r_{ij} \leq r_{cut} \\ 0 & \text{for } r_{ij} > r_{cut} \end{cases} \quad (11)$$

where  $r_{ij}$  is the separation distance between particle  $i$  and  $j$ ,  $d = (r_{ij} - r_0)$ ,  $\alpha$  and  $\varepsilon$  are parameters with dimensions of reciprocal distance and energy, and  $r_0$  is the equilibrium distance between two particles.

A mesoscale model was generated for HMX ([CH2-N(NO2)]4), where one mesoparticle was chosen to represent a single HMX molecule. Potential parameters were determined by analytical solution of the Morse potential expression, where the cohesive energy, density, and bulk modulus at zero temperature and pressure are the inputted observables. Following this procedure, we found  $\varepsilon=3440$  K,  $r_0=7.185$  Å, and  $\alpha=1.12$  Å<sup>-1</sup>. Further details for determining the Morse parameters can be found elsewhere [14]. For this HMX mesoscale model, good agreement was found for both the EOS properties and the elastic coefficients.

### Mesoparticle Equation of State

From statistical thermodynamics, the internal particle energy of an isolated non-linear polyatomic molecule containing  $n$  number of atoms can be expressed as the sum of the translational, rotational, vibrational, and electronic contributions, respectively, so that

$$\frac{u}{k_B T} = \frac{3}{2} + \frac{3}{2} + \sum_{j=1}^{3n-6} \left( \frac{\Theta_{vib,j}}{2T} + \frac{\Theta_{vib,j}/T}{e^{\Theta_{vib,j}/T} - 1} \right) - \frac{D_e}{k_B T} \quad (12)$$

where  $k_B$  is the Boltzmann constant,  $T$  is the temperature,  $\Theta_{vib,j}$  is the characteristic vibrational temperature and  $D_e$  is the depth of the ground electronic state potential well [15], both of which can be determined from quantum mechanics calculations or taken from thermodynamic tables [15] when available. As a first approximation for this study, we formulate Equation (12) based upon the classical limit (relatively high temperature), so that

$$\frac{u}{k_B T} = \frac{3}{2} + \frac{3}{2} + (3(28) - 6) = 81 \quad (13)$$

since each HMX molecule contains 28 atoms and is represented by a single mesoparticle. By

replacing  $T$  with the internal particle temperature  $\theta_i$ , we arrive at the equation of state for particle  $i$

$$\theta_i = \frac{u_i}{81k_B} \quad (14)$$

A sample configuration just prior to the release of elastic energy for this HMX model under shear is shown in Figure 3.

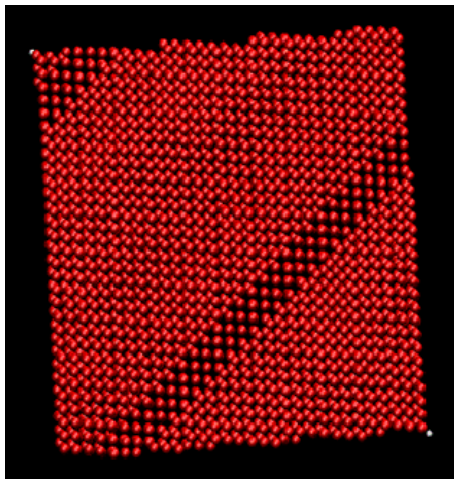


Fig. 3. Sample DPD-E simulation configuration of sheared material just prior to release of elastic energy.

### Verification of Approach

A benchmark problem is selected to demonstrate the concept of our algorithm. The simulation represents a hypothetical scenario to demonstrate the depiction of a reaction event that previously was unattainable. The lower part of a block (Figure 4) is initialized with a given velocity, while the upper part remains at rest to generate a predictable location of shear along the sliding surface. A standard explosive is chosen to verify the algorithm. Mie-Grüneisen and JWL equations of state are used for the reactant and products respectively.

In order to verify our model, we considered two different temperature values to represent two different shear rates. The time series of contours of extent of reaction illustrating a representative

low shear rate that corresponds to a temperature value of 500K is shown in Figure 5 (a). An insignificant rise in internal energy due to plastic work is observed. A pressure wave, albeit weak in strength, travels away from the shear localization. For the idealized scenario shown here, one would expect convection and boundary conditions to quickly prevent any form of a thermal runaway. Figure 5 (b) depicts a much more intense situation, where the temperatures in the localized region are much higher (1200K) and the energetic material along the shear surface is completely reacted, causing further increase in temperatures and pressures.



Fig. 4. Illustration of the initial condition for a benchmark shear initiated reaction problem.

### Concluding Remarks and Future Work

A newly developed multi-scale approach that includes a physics-based sub-grid model employing chemical kinetics for simulating shear initiated reactions is discussed. The details of the continuum, sub-grid, and mesoscale level simulations are provided. The approach is implemented into an Eulerian hydrocode and a benchmark verification exercise demonstrated that the new approach allows for simulations that were not previously possible for energetic materials when subjected to loads that result in shear localizations. This computational tool provides a novel modeling capability that opens previously unavailable avenues by bridging the gaps between multiple scales to enable improved predictions towards designing armor and anti-armor devices, and the development of concepts for enhanced survivability and lethality, primarily in the areas of insensitive munitions, reactive armor, and the development of novel concepts and designs utilizing reactive materials. Future developments in mesoscale modeling, and refinements at the sub-grid and continuum levels would undoubtedly

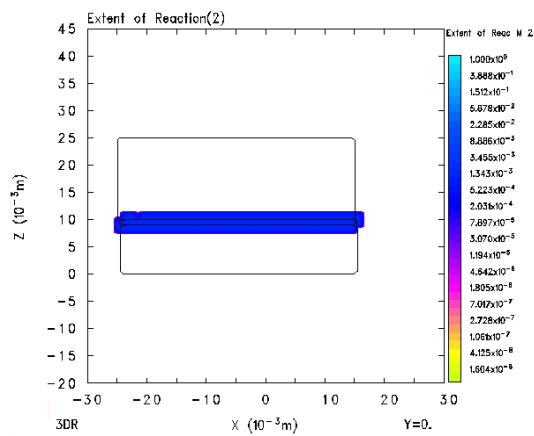
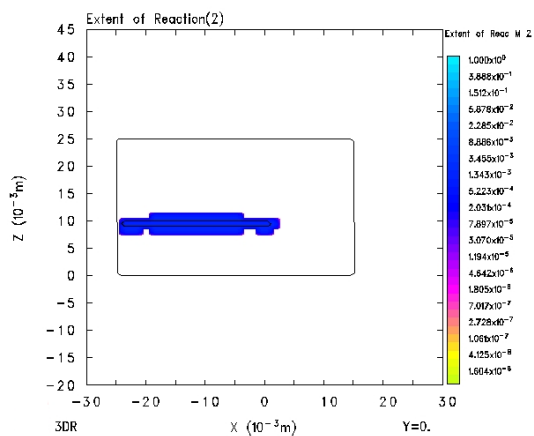
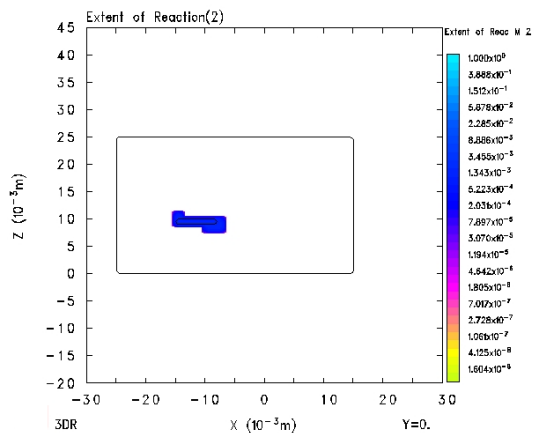


Figure 5(a). Time sequence of extent of reaction contour corresponding to a representative low shear rate

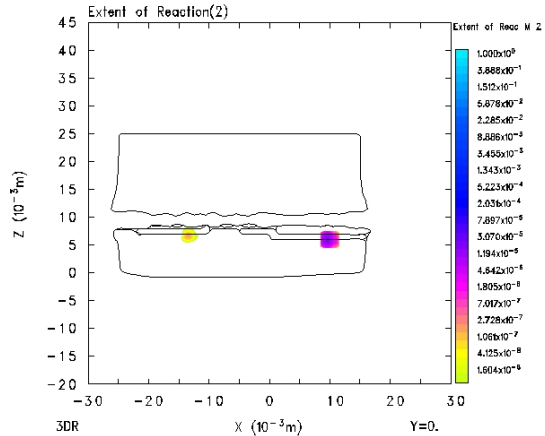
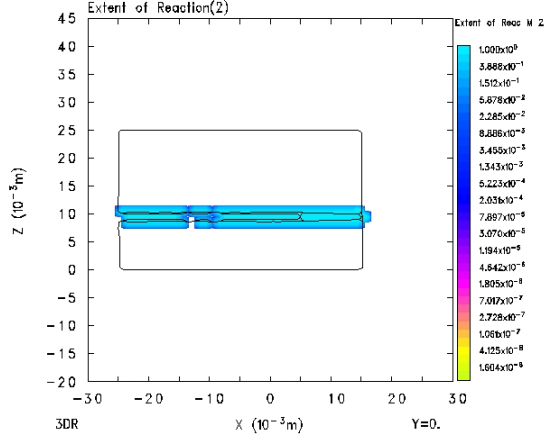
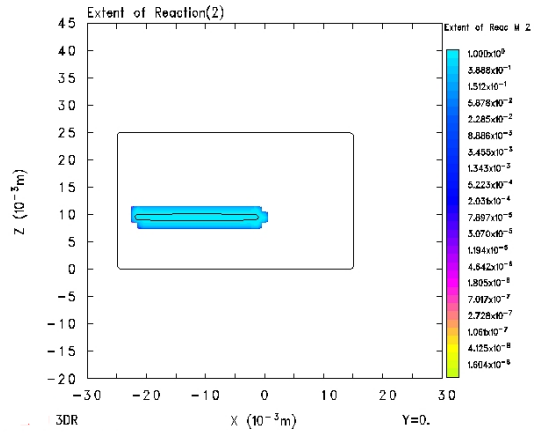


Figure 5(b). Time sequence of extent of reaction contour corresponding to a representative high shear rate

result in an improved predictive capability.

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